Hydrogen cyanide

74-90-8 | DTXSID9024148

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -9.25 °C

Global applicability domain: Inside

Local applicability domain index: 4.00e-01

Confidence level: 4.49e-01

Nearest Neighbors from the Training Set

Image not found
Hydrogen cyanide
Measured: -13.4
Predicted: -9.25

Image not found
Methyl isocyanide
Measured: -45.0
Predicted: -35.1

Image not found
2-Fluoroethanol
Measured: -26.4
Predicted: -20.0

Image not found
N-Hydroxy-N,N-dimethylamine
hydrochloride
Measured: 108
Predicted: 96.7

Image not found
N,N-Diethylhydroxylamine
Measured: 10.0
Predicted: 22.1